October 1974 LRP 87/74

T H A L I A

A ONE-DIMENSIONAL MAGNETOHYDRODYNAMIC STABILITY PROGRAM USING THE METHOD OF FINITE ELEMENTS

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Nature of Physical Problem

The lifetime of a magnetically-confined plasma column depends critically on the growth rates of any unstable eigenmodes. The plasma is considered here as a one-component fluid described by the ideal one-dimensional MHD equations [1]. Purely oscillating or purely growing and damped modes can be studied by linearising these equations and perturbing an equilibrium state of the column. Not only the purely growing modes, i.e. the unstable eigenfunctions, but also stable, purely oscillating modes can be of interest [2]. THALIA has been written to find the whole spectrum from the variational principle [3].

Method of Solution

The linearized ideal one-dimensional MHD equations are treated in variational form [3] by the method of finite elements [4]. In order to describe certain features of the problem with sufficient accuracy, (for example: a displacement vector which satisfies $\operatorname{div} \vec{\xi} \simeq 0$ for the fixed boundary case) we perform a rather general transformation and choose our basis functions from a class able to represent $\operatorname{div} \vec{\xi} = 0$ everywhere. The eigenvalue problem $Ax = \omega^2 Bx$ is solved by SIVI, a subprogram of the band matrix library HYMNIA [5].

Typical Running Time

The time required is proportional to the number of intervals, to the number of wanted eigenvalues and to the number of iterations. A typical case with 100 intervals, 20 iteration steps takes about 10 seconds per eigenvalue.

Unusual Features of the Program

THALIA uses the CDC OLYMPUS package [6], and follows all prescriptions of the OLYMPUS system [7]. The code is written in STANDARD FORTRAN [8], except for the use of the input facility NAMELIST which is available on most computers, and is optimized for speed and memory requirements. Memory requirements are reduced by storing only half the band-width for the symmetric band matrices A and B. For detecting a singular A or a degenerate eigenvalue problem in SIVI a machine dependent parameter EPSMAC has to be defined. EPSMAC is set to be 10^{-12} for a CDC 6500.

References

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1. INTRODUCTION

THALIA is a one-dimensional stability program which treats the ideal MHD equations [1] by the method of Ritz-Galerkin [3]. Finite elements [2] are taken as basis functions. This program is used to determine the MHD instabilities of infinitely extended cylindrical plasmas confined by magnetic fields, which are of interest in practice because the life time of the plasma depends on the growth rate of such instabilities. Starting from an equilibrium, one looks at possible eigenmodes which can be pure oscillations (stable case), pure growing modes (unstable case), or purely damped modes.

The basic equations, equilibrium, boundary and regularity conditions of the problem are described in section 2. The representation of the displacement vector by a special class of finite elements [5] is described in section 3, together with the construction of the matrices A and B which define the eigenvalue problem $Ax = \omega^2 Bx$, solved by simultaneous inverse vector interation [6,7] by the band matrix package HYMNIA [8]. Section 4 describes the program flow and explains the various subroutines. It also presents a set of tests with their input and output, which are then discussed in more detail in section 5. In this section we also show how the program can readily be adapted to a variety of situations.

The structure of THALIA is based on the OLYMPUS package [9,10]. THALIA is written in STANDARD FORTRAN [11] apart from the use of the NAMELIST input facility. In order to facilitate reading of the program listing we refer to equation numbers by comments in the code, while in the write up we refer to decimally-numbered program subroutines as follows e.g. <3.2>. Intelligible choice of variable identifiers should also help to make the listing straightforward to read.

2. THE PHYSICAL PROBLEM

2.1 Basic Equations

Consider a small, time and space-dependent displacement $\vec{\xi}$ of a perfectly conducting fluid in magnetohydrostatic equilibrium. The equation of motion for $\vec{\xi}$ is given by [4]

$$\rho \frac{\partial^2 \vec{\xi}}{\partial t^2} = \vec{F}(\vec{\xi}) = \vec{\nabla}(\vec{\xi}\cdot\vec{\nabla}p + \gamma p \vec{\nabla}\vec{\xi}) + (\vec{\nabla}\times\vec{Q})\times\vec{B} + (\vec{\nabla}\times\vec{B})\times\vec{Q} \tag{1}$$

where $\vec{Q} = \vec{\nabla}\times(\vec{\xi}\times B)$. Here $\rho(\vec{r})$, $p(\vec{r})$ and $\vec{B}(\vec{r})$ denote the equilibrium mass density, pressure and magnetic field respectively. γ is the adiabaticity index. The equilibrium quantities satisfy the relation

$$(\vec{\nabla}\times\vec{B})\times\vec{B} = \vec{\nabla}p \tag{2}$$

If the magnetic field is assumed known, together with the pressure at the wall, the function $p(\vec{r})$ can be found by integrating this equation towards the axis.

One way to attack the stability problem in an axisymmetric infinitely long plasma is to look for normal mode solutions

$$\vec{\xi}(\vec{r},t) = \vec{\xi}(r)e^{i(\omega t + m\theta + kz)} \tag{3}$$

of equation (1).

Introducing the 3 components of $\vec{\xi}$: ξ_r ξ_θ and ξ_z, the Lagrangian reads [12]

$$\delta L = 2\pi\delta \int_{r_{in}}^{a} r dr \left\{ \Lambda\left(\xi_r, \frac{d\xi_r}{dr}\right) + \gamma_p \left| \eta + \frac{1}{\gamma} \frac{d}{dr}(r\xi_r) \right|^2 + \frac{k^2 r^2 + m^2}{r^2} \left| \zeta - \zeta_0\left(\xi_r, \frac{d\xi_r}{dr}\right) \right|^2 \right\}$$

$$- 2\pi a \frac{z(a)}{z'(a)} F^2(a) \delta \left|\xi_r(a)\right|^2 - 2\pi\omega^2 \delta \int_{r_{in}}^{a} \rho r dr \left\{ |\xi_r|^2 + |\xi_\theta|^2 + |\xi_z|^2 \right\} \tag{4}$$

where Z(r) is a solution of

$$\frac{d^2 z}{dr^2} + \frac{1}{r} \frac{dz}{dr} + \left(k^2 + \frac{m^2}{r^2}\right) z = 0 \tag{5}$$

such that $Z'(R) = 0$ <2.5>. Here, a and r_{in} are the outer and inner radius of the plasma column, R the distance of the conducting wall, δ the variation of a functional and

$$\Lambda\left(\xi_r, \frac{d\xi_r}{dr}\right) = \frac{1}{k^2 r^2 + m^2} \left| F \cdot r \frac{d\xi_r}{dr} + \left(k B_z - \frac{m}{r} B_\theta\right) \xi_r \right|^2 + \left[F^2 - 2 \frac{B_\theta}{dr} \frac{d}{dr}(r B_\theta) \right] \xi_r \tag{6}$$

$$\zeta_0\left(\xi_r, \frac{d\xi_r}{dr}\right) = \frac{r}{k^2 r^2 + m^2} \left[\left(k B_\theta - \frac{m}{r} B_z\right) r \frac{d\xi_r}{dr} - \left(k B_\theta + \frac{m}{r} B_z\right) \xi_r \right] \tag{7}$$

$$\eta = \frac{im}{r} \xi_\theta + i k \xi_z \tag{8}$$

$$\zeta = i \xi_\theta B_\theta - i \xi_z \tag{9}$$

$$F = k B_z + \frac{m}{r} B_\theta \,. \tag{10}$$

For the fixed boundary case, (the plasma is bounded by an impenetrable wall, i.e. at R = a), Z'(a) becomes 0 and we end up with the boundary condition

$$\xi_r(a) = \xi_r(R) = 0. \tag{11}$$

In addition (4) is constrained by the regularity conditions

$$\vec{\xi}\,(r=0) \;=\; \text{finite and unique} \tag{12}$$

or by

$$\vec{\xi}\,(r=r_{in}) = 0 \tag{13}$$

for hard core geometry.

In (4) ξ_r, ξ_θ, ξ_z can be taken real without loss of generality [12]. Note that the left and the right hand sides of (4) are proportional to the kinetic and the potential energy $< 3.2 >$ of the plasma respectively. From (4) it is self-evident that the operator $\vec{F}(\vec{\xi})$ (1) is self-adjoint. This is shown for the general case by Greene and Johnson [14]. Hence the eigenfrequencies ω^2 are real. The plasma is unstable when negative eigenvalues ω^2 exist. Note further that (4) only contains derivatives of the radial component ξ_r.

2.2 Normalization

We choose a natural system of units ($\mu_0 = 1$) in which the plasma pressure is expressed in terms of the magnetic pressure. For numerical reasons it is appropriate to normalize the equilibrium quantities in such a way that the growth rates or frequencies become of order unity (Table 1).

Table 1: Normalization

Position	$r_{ph} = a * r_{num}$
Displacement	$\xi_{ph} = a * \xi_{num}$
Wave-number	$k_{ph} = (1/a) * k_{num}$
Wave-number	$m_{ph} = m_{num}$
Fields	$B_{ph} = B_o * B_{num}$
Density	$\rho_{ph} = \rho_o * \rho_{num}$
Pressure	$p_{ph} = B_o^2 * p_{num}$
Frequency	$\omega_{ph}^2 = \frac{B_o^2}{\rho_o a^2} * \omega_{num}^2$

The subscripts ph, num denote the physical and numerical variables, and B_o and ρ_o represent a typical magnetic field strength and density respectively. In order to find an accurate class of basis functions in section 3, and to remove the apparent singularities induced in (4) by the cylindrical geometry, we perform a rather general transformation on our variational principle (4)

$$\vec{\eta} = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix} = U\vec{\xi} = \begin{pmatrix} r^{-\alpha} & 0 & 0 \\ br^{\beta} & \frac{1}{c}r^{-\gamma} & 0 \\ 0 & 0 & dr^{-\delta} \end{pmatrix} \begin{pmatrix} \xi_r \\ \xi_\theta \\ \xi_z \end{pmatrix} \qquad (14)$$

Transformation (14) is a simple generalisation of the transformations used in [5,15] and is used for programming the eigenvalue problem (4) in section 3.

2.3 Features of the Equations

Unstable modes in the fixed boundary case are found in the regions where (10) $F = \vec{k}\cdot\vec{B} = \frac{m}{r} B_\theta + k B_z \approx 0$ [5,16]. These unstable modes are almost incompressible, i.e. $\mathrm{div}\,\vec{\xi} \approx 0$. In the variational principle (4) on the right hand side the second term comes from $\mathrm{div}\,\vec{\xi}$. The first and the third term together contain $\vec{k}\cdot\vec{B}$ and $\mathrm{div}\,\vec{\xi}$ terms, except one negative contribution which give rise to instabilities. It is evident that these features force us to be able to represent $\vec{k}\cdot\vec{B}$ and $\mathrm{div}\,\vec{\xi}$ exactly.

3. NUMERICAL TREATMENT

3.1 Choice of Mesh

The eigenfunctions $\vec{\xi}(r)$ may be highly localized functions of r and it is then advisable to choose the space mesh to suit the eigenmode which is being examined. This is done in THALIA by specifying a positive definite weight function w(r) which defines the relative density of mesh points at each radial position. The mesh index n(r) is then found by summation over a preliminary finescale mesh:

$$n(r) = 1 + N\left\{\int_{r_{in}}^{r} w(r)\,dr \Big/ \int_{r_{in}}^{1} w(r)\,dr\right\} \qquad (15)$$

where N is the total number of mesh intervals required and r_{in} is the inner radius. From this function the positions r_n corresponding to integral values of n(r) are found by linear interpolation, and finally the interval mesh-points $r_{n+\frac{1}{2}}$ are also constructed.

The weight function w(r) is specified by a function subprogram <1.10>

```
FUNCTION WMESH(R,CONST,KCASE)                    (16)
```

Five arbitrary constants are provided for each case, which in the subprogram are referred to as C1, C2,... C5 for brevity and in NAMELIST are represented by an array CONMSH (MAXCON,MAXCAS), the standard dimensions being MAXCON = 5 (number of constants), MAXCAS = 10 (number of cases which can be tested in one run). The default setting is C1 = 1, C2 = C3 = ...C5 = 0, thus giving a uniform mesh. A standard choice of function

$$w(r) = C_1 + C_2 r + C_3 \exp\left[-(C_4 - r)^2 / C_5^2\right] \qquad (17)$$

is provided in the published version of THALIA, but if the user wishes to specify his own weight function he can do so by changing the appropriate card in WMESH and recompiling. The mesh is constructed by subroutine MESH <2.7>.

3.2 Equilibrium

The equilibrium functions B_z, B_θ/r and ς are defined in a similar way by function subprogram <1.9>

```
FUNCTION EFUNCT (R,CONST,KVAR,KCASE,KLOOP)       (18)
```

and again five arbitrary constants C1, C2,... C5 for each case are provided for each of the three variables. Table 2 explains how the scheme

is set up:

Table 2: Equilibrium

KVAR	Variable	Standard function	NAMELIST Variable	Default Values
1	B_z	Function e(r) (15)	CONBZ(MAXCON,MAXCAS)	$c_1 = 1$, $c_2 = c_5 = 0$
2	$B_{o/r}$	Function e(r) (16)	CONBTR(MAXCON,MAXCAS)	$c_1 = \ldots\ldots = c_5 = 0$
3	β	Function e(r) (17)	CONRO(MAXCON,MAXCAS)	$c_1 = 1$, $c_2 = p_w$ $c_3 = c_4 = c_5 = 0$

where:

$$e(r) = c_1 + c_2 \exp\left\{-\exp\left[(c_3 - r)/c_4\right]\right\} \tag{19}$$

$$e(r) = c_5 + \left\{c_1 + c_2 \exp\left[-(r - c_3)^2/c_4^2\right]\right\}/r^2 \tag{20}$$

$$e(r) = c_1 \left[p(r) / c_2\right] \tag{21}$$

We assume that the temperature is homogeneous, i.e. the density is proportional to the pressure. Knowing the field distributions (19), (20) and the wall pressure we integrate the pressure balance equation (2) inwards, as indicated below, and afterwards construct the density using (21). In definition of B_z and B_θ/r, c_3 describes the position of the localized properties, and c_4 their width. It is evident that c_3 and c_4 have to be chosen about the same, since otherwise it will not be possible to obtain a physical pressure which is positive everywhere.

The user can specify his own functions by changing the appropriate cards in EFUNCT and recompiling. This is likely to be necessary if the equilibrium is determined from experimentally-measured values, e.g. by means of a least-square fit.

Given the pressure p_w at the wall (r = 1), the function (r) can be found by inward integration of equation (2) in the form

$$\frac{\partial p}{\partial r} = -B_z \frac{\partial B_z}{\partial r} + r \frac{B_\theta}{r}\left[r \frac{\partial}{\partial r}\left(\frac{B_\theta}{r}\right) + 2\left(\frac{B_\theta}{r}\right)\right] \qquad (22)$$

The derivatives are found by numerical differentiation over a small radial interval $\Delta r = \pm 10^{-3}$, and therefore the functions (19) and (20) must be continuous and analytically defined beyond the endpoints (r_{in}, 1). The wall pressure p_w is specified by NAMELIST variable CONPWL (MAXCAS) with default value $p_w = 0.05$. The equilibrium is constructed by subroutine EQUIL <2.3> .

3.3 Finite Elements

The variational principle (4) is solved by the method of Ritz-Galerkin [3]. Finite elements are taken as basis functions. In order to find the best approximating elements we perform a radius-dependent transformation (14) on the eigenvectors. The expansion of the transformed vector $\vec{\eta}$ in finite elements is given by

$$\vec{\eta}(r) = \begin{pmatrix} \eta_1(r) \\ \eta_2(r) \\ \eta_3(r) \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{N_r} R_i\, r_i(r) \\ \sum_{i=1}^{N_\theta} \theta_i\, t_i(r) \\ \sum_{i=1}^{N_z} Z_i\, z_i(r) \end{pmatrix} \qquad (23)$$

where the elements are denoted by $r_i(r)$, $t_i(r)$ and $z_i(r)$ and the expansion coefficients by R_i, θ_i, Z_i. Note that the numbers N_r, N_θ and N_z may differ by 1, if a mixture of linear (hat function) and constant (towar function) elements [5] is used.

Let us define

$$\vec{x}^T = (R_1, \theta_1, z_1, R_2, \theta_2, z_2, \ldots) \equiv (x_1, \ldots, x_n) \tag{24}$$

where $n = N_r + N_\theta + N_z$ is the total number of vector components. The variational form of Hamilton's principle (4) can then be written in the form

$$\omega^2 \sum_{k=1}^{n} \left(\int_{r_{in}}^{1} B_{lk}(r)\,dr \right) x_k = \sum_{k=1}^{n} \left(\int_{r_{in}}^{1} A_{lk}(r)\,dr \right) x_k \quad , l = 1, \ldots, n \tag{25}$$

When we choose hat functions to represent all components (23), and for the transformation U = 1, we obtain the same problem as was solved in [18].

3.4 Choice of Transformation and Elements

In (2.3) we discussed the features of (4) and found that $\vec{k}\cdot\vec{B}$ and $\operatorname{div}\vec{\xi}$ [5,16] have to be represented exactly. In the one-dimensional case $\vec{k}\cdot\vec{B}$ is defined only by the equilibrium, and has no influence on the choice of basis functions. Let us examine $\operatorname{div}\vec{\xi}$:

$$\operatorname{div}\vec{\xi} = \frac{1}{r}\frac{d}{dr}(r\xi_r) + \frac{m}{r}\xi_\theta + k\xi_z = \frac{d\xi_r}{dr} + \frac{\xi_r + m\xi_\theta}{r} + k\xi_z \tag{26}$$

where the phases $\frac{\pi}{2}$ have been incorporated in ξ_θ and ξ_z [12].

We use the following transformation for $m \neq 0$:

$$\vec{\eta} = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix} = U\vec{\xi} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{r} & \frac{m}{r} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \xi_r \\ \xi_\theta \\ \xi_z \end{pmatrix} \tag{27}$$

which transforms div $\vec{\xi}$ into

$$\operatorname{div}\vec{\xi} = \frac{d\eta_1}{dr} + \eta_2 + k\eta_3 . \tag{28}$$

This transformation corresponds to the default values for $m \neq 0$ in the code <2.2>. The transformation parameters in (14) become $\alpha = 0$, $\beta = -1$, $\gamma = 1$, $\delta = 0$, $b = 1$, $c = \frac{1}{m}$, $d = 1$.

For $m = 0$ we choose another transformation which describes the div $\vec{\xi}$ accurately:

$$\alpha = -1 , \beta = 0, \gamma = 0 , \delta = -1 , b = 0 = d = 1 . \tag{29}$$

The choice of elements is now very simple: η_1 is represented by hat functions (whose derivatives are tower functions in an interval), η_2 and η_3 are represented by tower functions. The expansion coefficients R_i of the η_1's in (16) are defined on mesh points, θ_i and Z_i, the expansion coefficients of η_2 and η_3, are defined in the center of the intervals. With this choice of elements the numbers N_r, N_θ and N_z (15) satisfy the conditions $N_R = N_\theta + 1$ and $N_\theta = N_z$.

3.5 Interval Contribution $\mathcal{A}$ and $\mathcal{B}$

The matrices A and B (25) can be written in terms of partial matrices $\mathcal{A}_i$ <2.10> and $\mathcal{B}_i$ <2.11>. These matrices contain all function cross products of one interval i. They are given by (30) and (31).

$$\mathcal{A}_i \quad (30)$$

$f_{11}q_{11}+f_{14}q_{14}+f_{41}q_{41}+f_{44}q_{44}$	$f_{12}q_{12}+f_{42}q_{42}$	$f_{13}q_{13}+f_{43}q_{43}$	$f_{11}q_{15}+\frac{1}{2}(f_{14}+f_{41})(q_{18}+q_{45})+f_{44}q_{48}$	$f_{12}q_{16}+f_{42}q_{46}$	$f_{13}q_{17}+f_{43}q_{47}$
$f_{21}q_{21}+f_{24}q_{24}$	$f_{22}q_{22}$	$f_{23}q_{23}$	$f_{21}q_{25}+f_{24}q_{28}$	$f_{22}q_{26}$	$f_{23}q_{27}$
$f_{31}q_{31}+f_{34}q_{34}$	$f_{32}q_{32}$	$f_{33}q_{33}$	$f_{31}q_{35}+f_{34}q_{38}$	$f_{32}q_{36}$	$f_{33}q_{37}$
$f_{11}q_{51}+\frac{1}{2}(f_{41}+f_{14})(q_{81}+q_{54})+f_{44}q_{84}$	$f_{12}q_{52}+f_{42}q_{82}$	$f_{13}q_{53}+f_{43}q_{83}$	$f_{11}q_{55}+f_{14}q_{58}+f_{41}q_{85}+f_{44}q_{88}$	$f_{12}q_{56}+f_{42}q_{86}$	$f_{13}q_{57}+f_{43}q_{87}$
$f_{21}q_{61}+f_{24}q_{74}$	$f_{22}q_{62}$	$f_{23}q_{63}$	$f_{21}q_{64}+f_{24}q_{68}$	$f_{22}q_{66}$	$f_{23}q_{67}$
$f_{31}q_{71}+f_{34}q_{74}$	$f_{32}q_{72}$	$f_{33}q_{73}$	$f_{31}q_{74}+f_{34}q_{78}$	$f_{32}q_{76}$	$f_{33}q_{77}$

$$\mathcal{B}_i \quad (31)$$

$g_{11}\,\mathcal{S}\,q_{11}$	$g_{12}\,\mathcal{S}\,q_{12}$	0	$g_{11}\,\mathcal{S}\,q_{15}$	$g_{12}\,\mathcal{S}\,q_{16}$	0
$g_{21}\,\mathcal{S}\,q_{21}$	$g_{22}\,\mathcal{S}\,q_{22}$	0	$g_{21}\,\mathcal{S}\,q_{25}$	$g_{22}\,\mathcal{S}\,q_{26}$	0
0	0	$g_{23}\,\mathcal{S}\,q_{33}$	0	0	$g_{33}\,\mathcal{S}\,q_{37}$
$g_{11}\,\mathcal{S}\,q_{51}$	$g_{12}\,\mathcal{S}\,q_{52}$	0	$g_{11}\,\mathcal{S}\,q_{55}$	$g_{12}\,\mathcal{S}\,q_{56}$	0
$g_{21}\,\mathcal{S}\,q_{61}$	$g_{22}\,\mathcal{S}\,q_{62}$	0	$g_{21}\,\mathcal{S}\,q_{65}$	$g_{22}\,\mathcal{S}\,q_{66}$	0
0	0	$g_{33}\,\mathcal{S}\,q_{73}$	0	0	$g_{33}\,\mathcal{S}\,q_{77}$

where:

$$f_{11} = r^{2\alpha+1}\left\{\frac{1}{r^2}\left(B_z^2+\Gamma_p\right)\left[\alpha+1-bcmr^{\beta+\gamma}\right]^2+\left[(\alpha-1)\frac{B_\theta}{r}+bckB_z r^{\beta+\gamma}\right]^2+\right.$$
$$\left.+\left(kB_z+\frac{mB_\theta}{r}\right)^2-4\left(\frac{B_\theta}{r}\right)^2-2\,\frac{B_\theta}{r}\,r\,\frac{d}{dr}\left(\frac{B_\theta}{r}\right)\right\}$$

$$f_{12} = cr^{\alpha+\gamma+1}\left\{\frac{m}{r^2}\left(B_z^2+\Gamma_p\right)\left[\alpha+1-bcmr^{\beta+\gamma}\right]-B_z k\left[(\alpha-1)\frac{B_\theta}{r}+bckB_z r^{\beta+\gamma}\right]\right\}$$

$$f_{13} = dr^{\alpha+\delta+2}\left\{\frac{1}{r^2}\left(\Gamma_p k-\frac{B_\theta}{r}mB_z\right)\left[\alpha+1-bcmr^{\beta+\gamma}\right]+\frac{B_\theta}{r}k\left[(\alpha-1)\frac{B_\theta}{r}+bckB_z r^{\beta+\gamma}\right]\right\}$$

$$f_{14} = r^{2\alpha+2}\left\{\frac{1}{r^2}\left(B_z^2+\Gamma_p\right)\left[\alpha+1-bcmr^{\beta+\gamma}\right]+\frac{B_\theta}{r}\left[(\alpha-1)\frac{B_\theta}{r}+bckB_z r^{\beta+\gamma}\right]\right\}$$

$$f_{22} = c^2 r^{2\gamma-1}\left\{\Gamma_p m^2+\left(k^2r^2+m^2\right)B_z^2\right\} \qquad (32)$$

$$f_{23} = cdr^{\gamma+\delta}\left\{\Gamma_p mk-\left(k^2r^2+m^2\right)\frac{B_\theta}{r}B_z\right\}$$

$$f_{24} = cr^{\alpha+\gamma}\left\{\Gamma_p m-\left(krB_\theta-mB_z\right)B_z\right\}$$

$$f_{33} = d^2 r^{2\delta+1}\left\{\Gamma_p k^2+\left(k^2r^2+m^2\right)\left(\frac{B_\theta}{r}\right)^2\right\}$$

$$f_{34} = dr^{\alpha+\delta+1}\left\{\Gamma_p k+\left(krB_\theta-mB_z\right)\frac{B_\theta}{r}\right\}$$

$$f_{44} = r^{2\alpha+1}\left\{B_z^2+B_\theta^2+\Gamma_p\right\}$$

and

$$
\begin{aligned}
q_{11} &= r^{2d+1} \left\{1 + c^2 b^2 r^{2\beta+2\gamma}\right\} \\
q_{12} &= -bc^2 r^{d+\beta+2\gamma+1} \\
q_{22} &= c^2 r^{2\gamma+1} \\
q_{33} &= d^2 r^{2\delta+1}
\end{aligned}
\tag{33}
$$

The factors $q_{\mu\nu}$ <2.12> for any interval are the cross products of the basic functions and are determined by:

$$q_{\mu\nu} = e_\mu \cdot e_\nu \quad , \mu, \nu = 1, \ldots, 8 \tag{34}$$

where

$$\vec{e} = \left(r_i, t_i, z_i, r_i', r_{i+1}, t_{i+1}, z_{i+1}, r_{i+1}'\right) \tag{35}$$

and $' = \frac{d}{dr}$.

3.6 Integration by Simpson's rule

Summation over all intervals < 2.4 > of the integrated interval contributions $\mathcal{A}_i$ and $\mathcal{B}_i$ leads to an eigenvalue problem

$$A\vec{x} = \omega^2 B\vec{x} \tag{36}$$

where

$$
\begin{aligned}
A &= \sum_{i=1}^{N} \int_{r_{i-1}}^{r_i} \mathcal{A}_i \, dr \\
B &= \sum_{i=1}^{N} \int_{r_{i-1}}^{r_i} \mathcal{B}_i \, dr
\end{aligned}
\tag{37}
$$

These integrations < 2.9 > are performed by Simpson's rule [19]. In the eigenvalue problem (36) $\vec{x}$ denotes the displacement vector (24) and ω^2 the corresponding eigenvalue. Positive ω^2 gives rise to a pure oscillation, negative ω^2 is equivalent to a growth rate $\Gamma^2 = -\omega^2$.

Note that in THALIA the eigenvector $\vec{\xi}$ is normalized in such a way that

$$\int_{r_{in}}^{1} r dr \left|\vec{\xi}\right|^2 = 1$$

3.7 Eigenvalue Problem

The eigenvalue problem (36) is solved by simultaneous inverse vector iteration [6,7], for which we use the subprogram SIVI of the band matrix package HYMNIA [8]. The band features of A and B are conserved during all calculations, and the decomposition of A and B is carried out within the arrays A and B themselves, this saving storage space. Only the lowest absolute eigenvalues can be obtained. In order to find an arbitrary eigenvalue one shifts the problem by a suitable quantity ω_0^2 and solves

$$(\tilde{A} - \tilde{\omega}^2 B)\vec{x} = 0 \qquad (38)$$

where $\tilde{A} = A - \omega_0^2 B$ and $\tilde{\omega}^2 = \omega^2 - \omega_0^2$.

The number of eigenvalues less than ω_0^2 is calculated by SIVI. It is therefore always possible to know if one has missed an eigenvalue or not and the most unstable mode can also be obtained with confidence.

Section (5.1) describes how the library package HYMNIA is loaded. SIVI is called in < 2.1 >

```
CALL SIVI (A,B,X,U,V,AL,CONV,EPSCON,EPSMAC,NPIN,NPOUT)          (39)
```

The meanings of the formal parameters are described in Table 3.

Table 3: Parameters of SIVI

A [18 * (N+1)]	I/O	Potential energy matrix
B [18 * (N+1)]	I/O	Kinetic energy matrix
X [3 * NKV * (N+1)]	0	NKV eigenvectors sequentially stored
U [3 * NKV * (N+1)]	0	"Eigenvalue vector"
V [3 * NKV * (N+1)]		Working space
AL [NKV]	0	NKV eigenvalues
AL (1)	I	Shifting eigenvalue
CONV [NITMAX]	0	Convergence vector
EPSCON	I	Accuracy of the eigenvector
EPSMAC	I	Machine accuracy
NPIN [7]	I	Input parameters
NPIN (1) = 0	I	Vector iteration required
NPIN (2) = 3*(N+1)	I	Matrix length
NPIN (3) = 6	I	Half band width
NPIN (4) = NKV	I	Number of simultaneous iterated vectors
NPIN (5) = NITMAX	I	Maximum number of iteration steps
NPIN (6) = NSAVE	I	Channel number for saving, A, B on disk
NPIN (7) = NOUT	I	Channel for output
NPOUT [5]	0	Output parameters
NPOUT (1) = NEG	0	Number of eigenvalues less than ω_0^2
NPOUT (2) = NIT	0	Number of iterations
NPOUT (3) = NCONV	0	Number of converged vector components
NPOUT (4) = 0/-1	0	B is positive / not positive
NPOUT (5) = 0/-1	0	A is regular / singular

3.8 Boundary and Regularity Conditions

3.8.1 Fixed boundary case

The boundary condition <2.5> for a cylindrical pinch (4) and for $a \leq R$ is given by

$$\eta_1 (r=1) = \xi_r (r=1) = 0 \tag{40}$$

In THALIA these conditions are imposed by replacing the corresponding rows and columns in A and B by unit vectors <2.8>. The diagonal values are chosen to be 1 and 10^{-20} for A and B respectively. What in fact we are doing is to introduce a very high eigenvalue 10^{20} in order to delete a row and a column. The advantage is that we neither need to rearrange the matrices before calling SIVI nor to reintroduce the boundary conditions afterwards.

3.8.2 Free boundary case

The Lagrangian (5) contains a vacuum energy contribution <2.14>

$$\text{CONVAC} = -2\pi a \frac{z(a)}{z'(a)} F^2(a) \left| \xi_r(a) \right|^2 , \tag{41}$$

where Z(a) and Z'(a) are obtained by integrating (6) by the method of Runge-Kutta-Merson [20] <2.15>.

3.8.3 Regularity conditions

With (27) and (29) conditions (12) can be written as:

$$
\begin{aligned}
|m| &= 0 \quad : \eta_1 = \eta_2 = \eta_3 = 0 \\
|m| &= 1 \quad : \eta_1, \eta_2 \text{ finite} ; \eta_3 = 0 \\
|m| &> 1 \quad : \eta_2 \text{ finite} ; \eta_1 = \eta_3 = 0
\end{aligned}
\tag{42}
$$

In order to impose vanishing η-components in conditions (42) we proceed in the same way as for the boundary conditions, striking away a row and a column by introducing a new but very high eigenvalue $\langle 2.8 \rangle$.

3.8.4 Hard core geometry

For a hard core geometry we apply the condition of an impenetrable wall at inner radius r_{in}:

$$
\eta_1 (r = r_{in}) = r_{in}^{-d} \, \xi_r (r = r_{in}) = 0 \tag{43}
$$

4. THE COMPUTER CODE

4.1 Program Structure

The THALIA stability code comprises a main program and 119 subprograms of which 51 are part of the CDC Cyber 7326 Scope 3.4.2 system library. 12 subprograms are part of the HYMNIA band matrix package which is used to solve the eigenvalue problem (30). The user library CRONUS contains 26 subroutines.

File THALIA itself consists of the main program and 30 subprograms. The loading of all these utilities and a list of THALIA subprograms are described in section 5.1, where we give the so-called day-file (Fig. 2), showing how the control cards are processed. The flow diagram for THALIA is presented in Fig. 1.

The variables used in THALIA are mainly stored in six COMMON blocks given in the Appendix. The use of a blank common is advantageous because it employs program space that was previously used by the loader.

Each of the 29 subprograms of THALIA is decimally numbered according to the conventions of [9,10]. All references in this paper of the type <2.9> can be correlated with the subprogram index in the Appendix, and in Fig. 1. This index is also reproduced in the source deck. On the CDC Cyber 7326 we use the UPDATE facility and the corresponding *DECK name is denoted by C2S9 (class 2, subprogram 9).

4.2 Tests

Two tests are provided, the homogeneous θ-pinch and the homogeneous screw-pinch with a current that leads to an instability. Output from the second test is shown as TEST RUN OUTPUT. The θ-pinch test corresponds to the default option <1.2> of THALIA i.e. the problem given in Table 4 is solved if no input is given. The chosen transformation and the finite elements are those described in 3.4. With the default input we obtain one eigenvector of the degenerate Alfvèn class $\omega^2_{num} = k^2$ [15]. This class is determined by $\mathrm{div}\vec{\xi} = 0$ and $\xi_z = 0$. Because of N-fold degeneracy we can choose in one displacement direction an arbitrary function, e.g. ξ_r. The other direction, ξ_θ, is then defined by $\mathrm{div}\vec{\xi} = 0$. For the second test case, the homogeneous screw-pinch, we read the NAMELIST input variables

$$k_{num} = -0.2, \left(\frac{B_\theta}{r}\right)_{num} = 0.2, \left(\omega_0^2\right)_{num} = -3.10^{-4}, NKV = 2. \quad (44)$$

For these input variables we fulfil $\vec{k}\cdot\vec{B} = 0$ everywhere in the whole interval $0 \leq r \leq 1$. The analytically-determined two most unstable eigenvalues are $\omega^2_{num} = -3.87\cdot10^{-4}$ and $\omega^2_{num} = -1.15\cdot10^{-4}$ respectively. The eigenfunctions are approximately Bessel functions.

Further calculations can be found in [5] where we present the whole spectrum of a θ-pinch, the spectrum of the incompressible screw-pinch and the possibility of recovering continuous spectra by THALIA. In [21] high m calculations for a diffuse hard core pinch using similar equilibria to those described in Table 2 are presented.

Table 4: Default Input

Number of intervals	n = 10
Mesh	equidistant
Wave number	$k_{num} = -0.5$
Wave number	$m_{num} = 1$
Field	$(B_z)_{num} = 1.0$
Field	$(B_\theta/r)_{num} = 0.0$
Density	$\rho_{num} = 1.0$
Pressure	$(p_w)_{num} = 0.05$
Adiabaticity	$\gamma = 5/3$
Number of vectors	NKV = 1
Frequency shift	$(\omega^2_0)_{num} = 0.25$

5. INSTRUCTIONS FOR THE USER

5.1 Loading

Fig. 2 contains the so-called day-file of a typical job. The third and

fourth line contain the job card followed by request to attach from the disk the three program section OLDPL (Fortran), and HYMNIA and CRONUS (binary libraries). OLDPL is then treated by the facility UPDATE, which creates a so-called COMPILE file prepared for FORTRAN compilation. Any temporary changes to the Fortran can be edited at this stage. The compilation then creates the binary file THALIA. The OLYMPUS package CRONUS and the band matrix package HYMNIA are declared as user libraries and a loading map is performed after the loading of THALIA which is subsequently executed.

The CDC version of the THALIA package which is available from the CPC Library is arranged to set up the facility described in this section.

5.2 Input / Output

The input of parameters to the calculation is done in subprogram DATA<1.4> by the NAMELIST facility which is not STANDARD FORTRAN [11], but is available on most computer systems. The variables and arrays contained in NAMELIST NEWRUN are listed in the Appendix. Generally, only the equilibrium and mesh quantities (CONBTR, CONBZ, CONPWL, CONRO, CONMSH), the eigenvalue shift $(\omega_0^2)_{num}$, γ, the inner radius, the m and k vectors, NITMAX, NMESH, NCASES and NKV have to be given. If NAMELIST facility is not available it is only necessary to replace the statement

```
READ (NREAD,NEWRUN)                                    (45)
```

in DATA by a normal FORTRAN READ statement, which includes all the variables of the NAMELIST. The NAMELIST input for the second test case is given in TEST RUN OUTPUT. The output has already partly been described in section 4.2. First one obtains the list of all input variables and arrays of NAMELIST NEWRUN which were introduced for the second test case, followed by the physical output.

5.3 Program Restrictions

1. Not more than 10 cases (MAXCAS = 10) can be run in one job.

2. The program allows at present at most 100 intervals (MAXCAL = 201, MAXSIZ = 303).

3. The maximum number of simultaneous iterated vectors cannot exceed MAX (10,100/N), (since MAXEIG = 10). Using 50 intervals, for example, only 2 eigenvectors can be iterated simultaneously.

4. The maximum number of iteration steps is currently 50 (MAXIT = 50).

5. The number of constants used to define the mesh ≺ 1.10 ≻ and the equilibrium < 1.9 > are restricted to 5 (MAXCON = 5).

6. The internal radius (axis) for cylindrical geometry cannot be $r_{in} = 0$ but is set to $r_{in} = 10^{-20}$ for numerical purposes (division by r).

7. EPSCON has a default value of EPSCON = 10^{-4}.

8. EPSMAC is put to EPSMAC = 10^{-12} for a CDC 6500. This parameter may have to be changed for another machine.

5.4 Program Modifications and Suggestions

With the UPDATE facility it is very simple to change THALIA. Changing the dimensions requires changing DIMENSION statements in the COMMON blocks [C2.1], [C2.2], [C3.1], [C9.0], and corresponding changes to variables MAX... in < 1.2 > . For another choice of transformation (27) and (29) the user has to take into account the regularity conditions (42) in ≺ 2.6 ≻. The restriction $r_{in} \geq 10^{-20}$ may conceivably cause some trouble (almost infinite matrix elements in the first interval).

Subprograms SIVI and ORNOS of the CPC library package HYMNIA call a system routine RANF(N) where N is a dummy argument. RANF is the CDC random number generator. On other systems it may be necessary to employ a corresponding routine with a different name.

We suggest that users of THALIA should iterate on only one eigenvector at a time, because the computer time depends about linearly on the number of iterated vectors and the number of iterations [8]. Increasing the number of vectors increases both the number of iterations, and the computing time per eigenvalue. In order to find the right-shifting value $(\omega_0^2)_{num}$ we suggest doing some initial runs with small MAXIT, and localizing the wanted eigenvalue by the NEG (number of eigenvalues less then $(\omega_0^2)_{num}$)-facility. Simultaneous iterations of several eigenvectors should be done for finding the whole spectrum of a degenerate class. By doing a few iterations only over a few eigenvectors one can also obtain some information on where to find these modes.

This work was performed under the auspices of the Swiss National Science Foundation.

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APPENDIX

THALIA: Subprogram Names and Identification Numbers

Name	No	Number of arguments	Title
Class 1:	Prologue		
LABRUN	1.1		Label the run
CLEAR	1.2		Clear variables and arrays
PRESET	1.3		Set default values
DATA	1.4		Define data specific to run
AUXVAL	1.5		Set auxiliary values
EFUNCT	1.9	5	Define equilibrium functions
WMESH	1.10	3	Define equilibrium mesh
Class 2:	Calculation		
STEPON	2.1		Step on the calculation
SETPAR	2.2		Set parameters for new case
EQUIL	2.3		Construct equilibrium
CONMAT	2.4		Construct matrices A and B
BOUND	2.5		Apply boundary conditions
REGUL	2.6		Apply regularity conditions
MESH	2.7		Construct mesh
AWAY	2.8	1	Introduce very high eigenvalue
SIMINT	2.9	2	Simpson's integration for interval
AMTRX	2.10	2	Interval contribution for matrix A
BMTRX	2.11	2	Interval contribution for matrix B
SETQ	2.12		Construct the matrix Q
SYMTRZ	2.13	2	Symmetrize a square array
Class 3:	Output		
OUTPUT	3.1	1	Control the output
EPOT	3.2	6	Calculate potential energy
BACKTR	3.3	1	Transform back to ζ_r, ζ_θ, ζ_z
NORMLZ	3.4		Normalize
Class 5:	Diagnostics		
REPORT	5.1		Diagnostic reporting subroutine
CLIST	5.2	2	Print common variables
ARRAYS	5.3	2	Print common arrays
Class 0:	Control		
EXPERT	0.4		Modify standard operation of program
CRASH	0.5	3	Define CDC Scope recovery procedure

Name	No	Number of variables or arrays	Title
COMBAS	C1.1	25	Basic system parameters
COMDDP	C1.9	20	Development and diagnostic parameters
COMPHY	C2.1	10	General physical variables and arrays
COMEQU	C2.2	12	Equilibrium variables and arrays
COMNUM	C3.1	28	General numerical variables and arrays
COMADM	C4.1	3	Administrative variables
COMDIM	C4.2	14	Dimension parameters
(COMBLA)	C9.0	8	Blank common for matrix and vector storag

THALIA: List of the Variables and Arrays of the Namelist input Facility

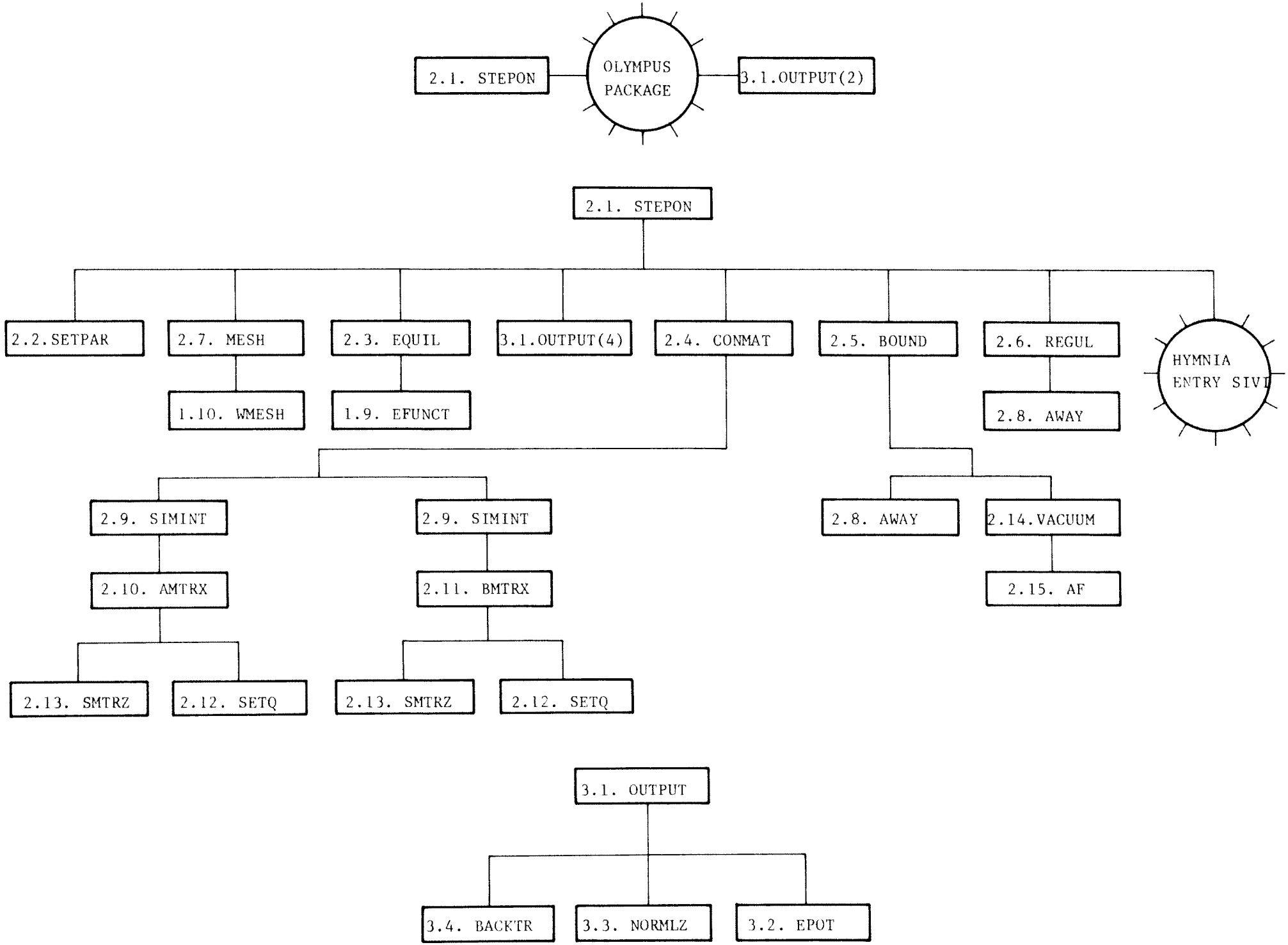
NEWRUN

Name/Length	type	Common block	Purpose
ALAM (MAXCAS)	RA	C3.1	Shift in eigenvalue
CONBTR (MAXCON,MAXCAS)	RA	C2.2	Constants for equilibrium B_θ/r
CONBZ (MAXCON,MAXCAS)	RA	C2.2	Constants for equilibrium B_z
CONMSH (MAXCON,MAXCAS)	RA	C2.2	Constants for weighting mesh
CONPWL (MAXCAS)	RA	C2.2	Wall pressure constants
CONRO (MAXCON,MAXCAS)	RA	C2.2	Constants for equilibrium density
EPSCON	R	C3.1	Convergence parameter
EPSMAC	R	C3.1	Machine accuracy
EPSPM (MAXCAS)	RA	C2.2	Defines preliminary mesh intervals
GAMMA	R	C2.1	Specific heat ratio
RIN (MAXCAS)	RA	C2.1	Inner radius in dimensionless units
WTM (MAXCAS)	RA	C2.1	M-value of wave or instability
WZK (MAXCAS)	RA	C2.1	K-value of wave or instability
MXDUMP	I	C1.9	See [10]
N	I	C3.1	Current number of radial intervals
NADUMP (20)	IA	C1.9	See [10]
NCASES	I	C1.1	See [10]
NIN	I	C1.1	See [10]
NITMAX	I	C3.1	Maximum number of iterations
NKV	I	C3.1	Number of eigenvalues required
NLEDGE	I	C1.1	See [10]
NMESH (MAXCAS)	IA	C3.1	Size of radial mesh n for each case
NONLIN	I	C1.1	See [10]
NOUP	I	C1.1	See [10]
NPDUMP (20)	IA	C1.9	See [10]
NPUNCH	I	C1.1	See [10]
NPRINT	I	C1.1	See [10]
NRUN	I	C1.1	See [10]
NSAVE	I	C4.1	Channel for saving matrices
NUDUMP (20)	IA	C1.9	See [10]
NLCHED	L	C1.9	See [10]
NLHEAD (9)	LA	C1.9	See [10]
NLOMT1 (50)	LA	C1.9	See [10]
NLOMT2 (50)	LA	C1.9	See [10]
NLOMT3 (50)	LA	C1.9	See [10]
NLREPT	L	C1.9	See [10]

FIGURE CAPTIONS

Fig. 1: Flow diagram of program THALIA.

Fig. 2: Day-file which shows loading of the three program sections HYMNIA, CRONUS and THALIA.


2.1. STEPON
OLYMPUS PACKAGE
3.1.OUTPUT(2)
2.1. STEPON
2.2.SETPAR
2.7. MESH
2.3. EQUIL
3.1.OUTPUT(4)
2.4. CONMAT
2.5. BOUND
2.6. REGUL
HYMNIA ENTRY SIVE
1.10. WMESH
1.9. EFUNCT
2.8. AWAY
2.9. SIMINT
2.9. SIMINT
2.8. AWAY
2.14.VACUUM
2.10. AMTRX
2.11. BMTRX
2.15. AF
2.13. SMTRZ
2.12. SETQ
2.13. SMTRZ
2.12. SETQ
3.1. OUTPUT
3.4. BACKTR
3.3. NORMLZ
3.2. EPOT

```
  EPF  LAUSANNE SCOPE3.4.2 LEV. 383   20/ 9/74
09.31.45.L085138  FROM
09.31.45.IP  00000256 WORDS - FILE INPUT  , DC 00
09.31.45.L0851,T100,CM77000.  GRUBER,CRPP
09.31.47.ATTACH(OLDPL,MHD,CY=2,ID=L0851,MR=1)
09.31.47.ATTACH(HYMNIA,JKMHD,CY=3,ID=L0852,MR=1)
09.31.47.
09.31.48.ATTACH(CRONUS,MHD,CY=4,ID=L0851,MR=1)
09.31.48.UPDATE(F,L=0)
09.32.06.  UPDATE COMPLETE.
09.32.06.FTN(I=COMPILE,B=THALIA)
09.34.35.     25.888 CP SECONDS COMPILATION TIME
09.34.35.MAP(PART)
09.34.35.LIBRARY(HYMNIA,CRONUS)
09.34.40.THALIA.
09.35.20.AUTOREL
09.36.38.     STOP
09.36.38.      5.466 CP SECONDS EXECUTION TIME
09.36.38.OP  00048832 WORDS - FILE OUTPUT , DC 40
09.36.38.CPA      19.633 SEC.          .654 ADJ.
09.36.38.CPB      20.125 SEC.          .670 ADJ.
09.36.38.IO       16.484 SEC.         1.098 ADJ.
09.36.38.CM     1673.275 KWS.        62.848 ADJ.
09.36.38.SS*** COUT DU CALCUL        65.20 FR ***
09.36.38.CO PERIPHERIE ET FACTEUR PRIORITE EN SUS
09.36.38.PP       52.204 SEC.      DATE 05/02/75
09.36.38.CC       30.60 FR I/O    0 PAUSES
09.36.38.EJ  END OF JOB, **


**********          L085138  //// END OF LIST ////
**********          L085138  //// END OF LIST ////
```

Fig. 2